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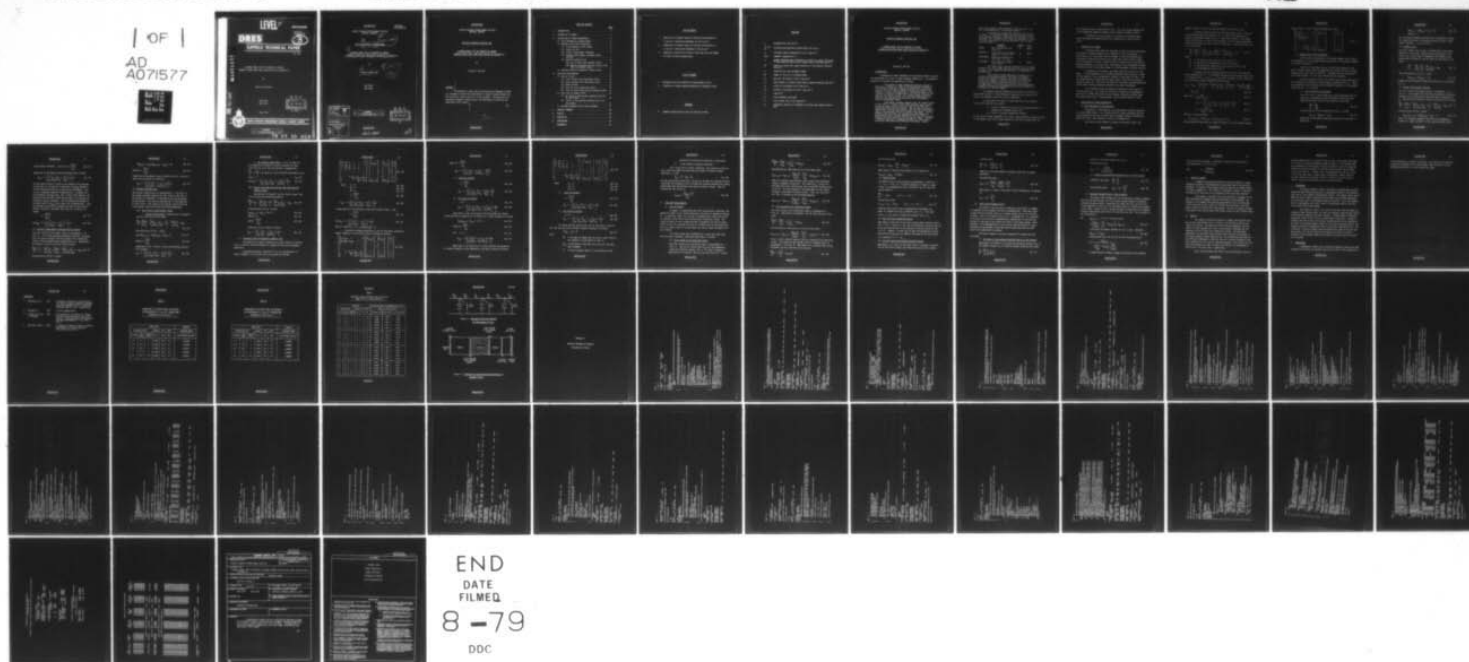
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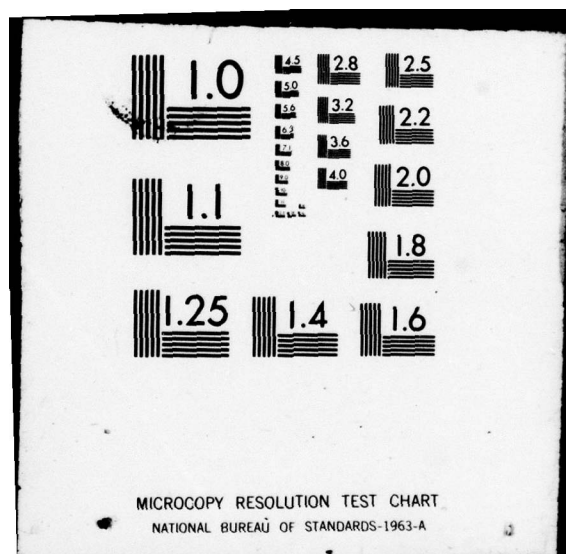
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A GENERAL MODEL FOR THE TRANSFER OF VAPOUR
THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING (U)

by

Stanley B. Mellisen

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A GENERAL MODEL FOR THE TRANSFER OF VAPOUR
THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING (U)

by

Stanley B. Mellisen

ABSTRACT

A mathematical model which was developed by Monaghan at DRES was extended to predict the penetration of vapour through clothed skin for an initial liquid load on or in the clothing. The model and its associated computer program along with some sample calculations are described in this report.

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NOTATION

a	decomposition rate (min^{-1})
A_i, B_i, C_i	diffusive and absorptive coefficients for slice i
C_s	saturated vapour concentration in air (mg cm^{-3})
DELT	computer language for Δt
g	general boundary term introduced to account for vapour evolution in the inward direction from a vapour-liquid interface (mg cm^{-2})
gf	same as g, except for vapour evolution in the outward direction (mg cm^{-2})
j	subscript for time increment number
MS	number of slices in a clothing layer
m_i	mass per unit area in slice i (mg cm^{-2})
Q	total amount of surface liquid lost to vapour evolution (mg cm^{-2})
R_a	diffusive resistance of air (min cm^{-1})
R_i	diffusive resistance of slice i (min cm^{-1})
t	time (min)
Δt	time increment size (min)
U	total vapour loss to air (mg cm^{-2})
V_i	absorptive capacity of clothing or skin per unit area of slice i (cm)

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Stanley B. Mellisen

1. INTRODUCTION

A mathematical model (Monaghan) was developed at DRES to predict the penetration of liquid or vapour through clothed skin. The essential features of the model are described as follows:

The problem of agent penetration through clothed or bare skin is treated as a case of one-dimensional diffusion in a multilayer system where absorptive and diffusive properties may vary from one layer to another and agent may decay in the system as a result of decomposition. The flow of agent in such a system is analogous to the flow of heat through a series of slabs or the flow of current in a resistance-capacitance network when the resistance and capacitors are very numerous (Pattle and Monaghan, 1964).

Experimental evidence suggests that the simplest model for the skin is a system in which two absorbent layers overlay a sink for agent, and only the layer next to the sink has a significant diffusional resistance. The two layers are broadly identifiable with the horny surface layer and the transitional layer of the epidermis and are so named in the model. The live epidermis and the dermis are ignored since both present no appreciable barrier to agent penetration and the latter is perfused by the blood which acts as the sink for agent. Similarly a clothing layer can be represented simply by a layer with a significant absorbence and diffusional resistance. Decom-

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position of agent has been observed in both skin and cloth and is approximated by a first order reaction.

An electrical analogue was chosen as the basis of the model. The following table gives the analogues of electrical charge, potential, capacitance and resistance used in the model for a clothing or skin layer of thickness ℓ , with a diffusion coefficient D , that has absorbed a mass of agent per unit volume C .

	<u>ANALOGUE</u>	<u>SYMBOL</u>	<u>UNITS</u>
CHARGE	Mass absorbed per unit area = $C\ell$	m	mg/cm^2
POTENTIAL	Equilibrium concentration, vapour in air, $C_e = C/\beta$	C_e	mg/cm^3
CAPACITANCE	Absorptive capacity per unit area = $\beta\ell = m/C_e$	V	cm
RESISTANCE	Diffusional Resistance = $\ell/D\beta = \ell^2/DV$	R	min/cm

The coefficient β and the capacitance V are assumed constant for a given agent and layer, but may vary from layer to layer. This assumption implies that V is independent of concentration.

The problem of agent penetration through skin is solved by deriving equations of flow from an analogous electric R-C network, in which each layer is divided into a sufficient number of uniform slices normal to the flow of agent to provide the required accuracy of solution. The equations of flow form a set of first order differential equations for each case considered and are solved numerically by means of a digital computer.

The computer program (McPherson) was written to calculate an approximate solution to the differential equations and to set up the initial and boundary conditions of the simulations.

In this program the model is subdivided into five submodels, two of which simulate cases where:

- a) liquid is deposited on the top of the outside layer of clothing on a clothed person; and
- b) liquid is pressed through the clothing.

In the first of these submodels, the initial liquid loading is specified, and in the second, the initial liquid loading in the cloth is specified, but

both loadings cannot be specified at once. Also, the second submodel and its corresponding computer program did not produce reasonable results.

The objective of this paper is to describe an improved model which can handle the generalized initial condition of liquid on and in cloth.

2. FEATURES OF THE MODEL

The penetration model was developed in order to better understand the hazards to people posed by toxic chemicals in the liquid phase. In other words, this study deals with an attempt to describe mathematically the physical processes occurring, with time, when liquid droplets impact on the clothing of a person, or when liquid is forced into the clothing by applying pressure, e.g. by sitting. The passage of the contaminant through clothing and skin to the blood stream is a time dependent diffusion process.

In addition to the above, two other provisions are part of the model. If the challenge is to a clothing ensemble, then provision is made for the removal of this contaminated clothing at some point in time. This is accomplished by zeroing the mass that exists in each of the clothing layers at that time. Similarly, the model will simulate the decontamination of the outer clothing surface by zeroing the surface contaminant.

In its present form, the model can handle up to four layers of clothing over skin. Each layer of clothing is assumed to be homogeneous. The skin is divided into three distinct regimes, the horny surface layer, the transitional layer of the epidermis, and the blood stream (a sink).

3. CALCULATION OF VAPOUR PENETRATION

a) Basic Mathematical Relationships

Penetration is described by a one-dimensional diffusion equation in a multi-layer system, i.e. clothing and skin, where absorptive and diffusion properties may vary from one layer to another and mass absorbed may decay with time in the system as a result of decomposition.

Each layer of the system is divided into several slices, the

number of which is chosen to provide adequate computing accuracy.

A general expression for flow of agent vapour into a slice can be obtained by applying Kirchoff's law at a node in the analogous resistance capacitance network (Fig. 1). Note that Kirchoff's law states that at any junction in the circuit the total current flowing toward the junction must equal the total current flowing away. Considering flow into slice i we obtain:

$$\frac{dm_i}{dt} = \left(\frac{m_{i-1}}{V_{i-1}} - \frac{m_i}{V_i} \right) \frac{2}{R_{i-1} + R_i} + \left(\frac{m_{i+1}}{V_{i+1}} - \frac{m_i}{V_i} \right) \frac{2}{R_i + R_{i+1}} - am_i \quad (\text{Eq. 1})$$

where

- m_i is the mass per unit area in slice i (mg cm^{-2})
- R_i is the diffusive resistance of slice i (min cm^{-1})
- V_i is the absorptive capacity per unit area of slice i (cm)
- a is the decomposition rate (min^{-1})

A simple implicit difference method was used to solve the diffusion equation (Eq. 1). If we denote the mass per unit area of skin slice i at time $j\Delta t$ by $m_{i,j}$, and $m_{i,j+1}$ at the next increment of time, then Eq. 1 can be written in the following discretized form:

$$m_{i,j} = m_{i,j+1} - \left(\frac{m_{i-1,j+1}}{V_{i-1}} - \frac{m_{i,j+1}}{V_i} \right) \frac{2\Delta t}{R_{i-1} + R_i} - \left(\frac{m_{i+1,j+1}}{V_{i+1}} - \frac{m_{i,j+1}}{V_i} \right) \frac{2\Delta t}{R_i + R_{i+1}} + am_{i,j+1}\Delta t \quad (\text{Eq. 2})$$

$$\text{Now let } A_i = \frac{-2\Delta t}{V_i(R_i + R_{i+1})} \quad (\text{Eq. 3})$$

$$B_i = 1 + \left[\frac{1}{V_i} \left(\frac{2}{R_{i-1} + R_i} + \frac{2}{R_i + R_{i+1}} \right) + a \right] \Delta t \quad (\text{Eq. 4})$$

$$C_i = \frac{-2\Delta t}{V_i(R_{i-1} + R_i)} \quad (\text{Eq. 5})$$

Then Eq. 2 can be written:

$$A_{i-1}m_{i-1,j+1} + B_im_{i,j+1} + C_{i+1}m_{i+1,j+1} = m_{i,j} \quad (\text{Eq. 6})$$

Now the general expression for vapour diffusion in a skin-clothing system

with n slices is given in the following matrix form:

$$\begin{bmatrix} B_1 & C_2 & 0 & \dots & \dots & \dots & 0 \\ A_1 & B_2 & C_3 & 0 & \dots & \dots & \dots \\ 0 & A_2 & B_3 & C_4 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & A_n & B_{n-1} & C_n & \dots \\ 0 & \dots & \dots & 0 & A_{n-1} & B_n & \dots \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{n,j+1} \end{bmatrix} = \begin{bmatrix} m_{1,j} \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{n,j} \end{bmatrix} \quad (\text{Eq. 7})$$

b) Boundary and Initial Conditions

While the basic mathematics of the model appears quite simple, the elegance of it is attained through the control of the various boundary and initial conditions.

The initial conditions consist of the liquid loading on the outer clothing surface, and the magnitude and distribution of the liquid loading within each layer of clothing. The model does not allow gaps in the liquid loading. All the liquid loads must be contiguous.

Special conditions occur at the inside and outside boundaries of the clothed skin system and at liquid-vapour interfaces (Fig. 2). These are accounted for by modifying the corresponding equations in the general expression (Eq. 7) as follows:

(1) First equation in the system

The first slice in the clothed skin system represents the systemic sink, the potential and resistance of which are zero.

Applying Kirchoff's law for flow into the slice gives:

$$\frac{dm_1}{dt} = \frac{2m_2}{V_2 R_2} \quad (\text{Eq. 8})$$

Discretizing Eq. 8 in the same way as for Eq. 1 gives:

$$m_{1,j+1} + C_2 m_{2,j+1} = m_{1,j} \quad (\text{Eq. 9})$$

Comparison to the general expression given by Eq. 4 and Eq. 6 then gives:

$$B_1 m_{1,j+1} + C_2 m_{2,j+1} = m_{1j} + gF \quad (\text{Eq. 10})$$

where $B_1 = 1$

gF is a general boundary term which was introduced to account for vapour evolution in the outward direction from a liquid-vapour interface. In Eq. 10, $gF = 0$.

(2) Inside of skin

The first inside slice of skin is represented by the second equation in the system. Noting that the resistance of the first slice is zero since it represents the systemic sink, application of Kirchoff's law for flow into the second slice gives:

$$\frac{dm_2}{dt} = -\frac{2m_2}{V_2 R_2} + \left(\frac{m_3}{V_3} - \frac{m_2}{V_2} \right) \frac{2}{R_2 + R_3} + am_2 \quad (\text{Eq. 11})$$

Then discretizing as for Eq. 1 gives:

$$B_2 m_{2,j+1} + C_3 m_{3,j+1} = m_{2,j} \quad (\text{Eq. 12})$$

Comparison to the general expression given by Eq. 6 then shows

$$A_1 = 0.$$

(3) Inside liquid-vapour interface

The last inside slice without liquid is designated $i = nk$ (Fig. 2). The potential for flow from the adjacent liquid containing slice is given by the saturated vapour concentration, C_s . Application of Kirchoff's law for flow into slice nk gives:

$$\frac{dm_{nk}}{dt} = \left(\frac{m_{nk-1}}{V_{nk-1}} - \frac{m_{nk}}{V_{nk}} \right) \frac{2}{R_{nk-1} + R_{nk}} + \left(C_s - \frac{m_{nk}}{V_{nk}} \right) \frac{2}{R_{nk}} - am_{nk} \quad (\text{Eq. 13})$$

Discretizing as for Eq. 1 gives:

$$A_{nk-1} m_{nk-1,j+1} + B_{nk} m_{nk,j+1} = m_{nk} + g \quad (\text{Eq. 14})$$

where g is a general boundary term which was introduced to account for vapour evolution in the inward direction from a

liquid-vapour interface. In Eq. 14, $g = \frac{2C_s \Delta t}{R_{nk}}$ (Eq. 15)

Comparison to the general expression given by Eq. 6 gives:

$$B_{nk} = 1 + \left[\frac{1}{V_{nk}} \left(\frac{2}{R_{nk-1} + R_{nk}} + \frac{2}{R_{nk}} \right) + a \right] \Delta t \quad (\text{Eq. 16})$$

For the special case of liquid in the clothing slice adjacent to the skin, Eq. 15 and Eq. 16 show that g and B_{nk} become infinite because the outer skin slice has no resistance. This is not a reasonable physical representation. To adjust this, the assumption was made that, over a finite time interval, the clothing dries from the inside so that there is a non-zero resistance to vapour transport. This resistance was assumed to increase from 0 to R_{nk+1} with time as the clothing dries. Then the average value of the resistance was used in the discretization, so that for the outer skin slice Eq. 15 and Eq. 16 become:

$$g = \frac{2C_s \Delta t}{R_{nk+1}} \quad (\text{Eq. 17})$$

$$\text{and } B_{nk} = 1 + \left[\frac{1}{V_{nk}} \left(\frac{2}{R_{nk-1}} + \frac{2}{R_{nk+1}} \right) + a \right] \Delta t \quad (\text{Eq. 18})$$

(4) Outside liquid-vapour interface within clothing

The first outside slice without liquid is designated $i = n\ell$ (Fig. 2). As for the previously mentioned interface, the potential for vapour transport from the adjacent slice containing liquid is the saturated vapour concentration, C_s . Application of Kirchoff's law for flow into slice $n\ell$ gives:

$$\frac{dm_{n\ell}}{dt} = \left(C_s - \frac{m_{n\ell}}{V_{n\ell}} \right) \frac{2}{R_{n\ell}} + \left(\frac{m_{n\ell+1}}{V_{n\ell+1}} - \frac{m_{n\ell}}{V_{n\ell}} \right) \frac{2}{R_{n\ell} + R_{n\ell+1}} - am_{n\ell} \quad (\text{Eq. 19})$$

Discretizing as for Eq. 1 gives:

$$B_{nl,j+1} + C_{nl+1} m_{nl+1,j+1} = m_{nl,j} + gF \quad (\text{Eq. 20})$$

$$\text{where } gF = \frac{2C_s \Delta t}{R_{nl}} \quad (\text{Eq. 21})$$

Comparison to the general case by referring to Eq. 4 and Eq. 6 shows that the value B is given by:

$$B_{nl} = 1 + \left[\frac{1}{V_{nl}} \left(\frac{2}{R_{nl}} + \frac{2}{R_{nl} + R_{nl+1}} \right) a \right] \Delta t \quad (\text{Eq. 22})$$

(5) Outside clothing slice

The outside clothing slice is designated by $i = nn$ (Fig. 2). The vapour transport equation for this slice is the last in the system of n equations. Liquid may or may not be present on the surface. This must be accounted for in the equations for this slice. Also, there is the special case of only one slice without liquid, which must be treated separately.

(5a) Two or more slices without liquid

1. Liquid on the surface. Application of Kirchoff's law for flow into slice nn gives:

$$\frac{dm_{nn}}{dt} = \left(\frac{m_{nn-1}}{V_{nn-1}} - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn-1} + R_{nn}} + \left(C_s - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn}} - a m_{nn} \quad (\text{Eq. 23})$$

Discretizing as for Eq. 1 gives:

$$A_{nn-1} m_{nn-1,j+1} + B_{nn} m_{nn,j+1} = m_{nn,j} + g \quad (\text{Eq. 24})$$

$$\text{where } g = \frac{2C_s \Delta t}{R_{nn}} \quad (\text{Eq. 25})$$

Comparison to Eq. 4 and Eq. 6 gives the modified value of B as follows:

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn}} \right) + a \right] \Delta t \quad (\text{Eq. 26})$$

2. No liquid on the surface. In Eq. 23 there is zero potential in place of C_s and resistance for flow rate into the slice from the outside is changed from $\frac{R_{nn}}{2}$ to $\frac{R_{nn}}{2} + R_a$ where R_a is the diffusive resistance of air.

Then $g = 0$ (Eq. 27)

$$\text{and } B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn} + 2R_a} \right) + a \right] \Delta t \quad (\text{Eq. 28})$$

(5b) Special case when only one outside slice does not contain liquid

Application of Kirchoff's law for flow of vapour into slice nn gives the following equation:

$$\frac{dm_{nn}}{dt} = \left(C_s - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn}} + \left(0 - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn} + 2R_{a2}} - am_{nn} \quad (\text{Eq. 29})$$

Discretizing as for Eq. 1 gives:

$$B_{nn} m_{nn,j+1} = m_{nn,j} + gF + g \quad (\text{Eq. 30})$$

$$\text{where } g = 0 \quad (\text{Eq. 31})$$

$$\text{and } gF = \frac{2C_s \Delta t}{R_{nn}} \quad (\text{Eq. 32})$$

Comparison to Eq. 4 and Eq. 6 gives:

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn}} + \frac{2}{R_{nn} + 2R_a} \right) + a \right] \Delta t \quad (\text{Eq. 33})$$

c) Complete System of Equations in Matrix Form

The equations of vapour transport can now be written in the form of Eq. 7 with all the modifications to account for the various boundary conditions.

Considering boundary conditions (1) to (3) the equations of vapour transport in the inside slices are written as follows:

$$\begin{bmatrix} B_1 & C_2 & 0 & \dots & \dots & 0 \\ A_1 & B_2 & C_3 & 0 & \dots & \dots \\ 0 & A_2 & B_3 & C_4 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & 0 & A_{nk-1} & B_{nk-1} & C_{nk} \\ 0 & \dots & \dots & 0 & A_{nk-1} & B_{nk} \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nk,j+1} \end{bmatrix} = \begin{bmatrix} m_{1,j} \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nk,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ \dots \\ \dots \\ \dots \\ 0 \\ g \end{bmatrix} \quad (\text{Eq. 34})$$

$$\text{where } A_1 = 0 \quad (\text{Eq. 35})$$

$$B_1 = 1 \quad (\text{Eq. 36})$$

$$gF = 0 \quad (\text{Eq. 37})$$

$$g = \frac{2C_s \Delta t}{R_{nk}} \quad (\text{Eq. 38})$$

$$B_{nk} = 1 + \left[\frac{1}{V_{nk}} \left(\frac{2}{R_{nk-1} + R_{nk}} + \frac{2}{R_{nk}} \right) + a \right] \Delta t \quad (\text{Eq. 39})$$

except when the slice adjacent to the skin contains liquid. Then:

$$g = \frac{2C_s \Delta t}{R_{nk+1}} \quad (\text{Eq. 40})$$

$$\text{and } B_{nk} = 1 + \left[\frac{1}{V_{nk}} \left(\frac{2}{R_{nk-1}} + \frac{2}{R_{nk+1}} \right) + a \right] \Delta t \quad (\text{Eq. 41})$$

which is identical to Eq. 4 because $R_{nk} = 0$.

Considering boundary equations (4) and (5) the matrix system for vapour transport in the outside slices is written as follows:

$$\begin{bmatrix} B_{nl} & C_{nl+1} & 0 & \dots & \dots & 0 \\ A_{nl} & B_{nl+1} & C_{nl+2} & 0 & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & A_{nn-1} & B_{nn-1} & C_{nn} & \dots \\ 0 & \dots & 0 & A_{nn-1} & B_{nn} & \dots \end{bmatrix} \begin{bmatrix} m_{nl,j+1} \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nn,j+1} \end{bmatrix} = \begin{bmatrix} m_{nl,j} \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nn,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ \dots \\ \dots \\ \dots \\ 0 \\ g \end{bmatrix} \quad (\text{Eq. 42})$$

$$\text{where } gF = \frac{2C_s \Delta t}{R_{nl}} \quad (\text{Eq. 43})$$

$$B_{nl} = 1 + \left[\frac{1}{V_{nl}} \left(\frac{2}{R_{nl}} + \frac{2}{R_{nl} + R_{nl+1}} + a \right) \right] \Delta t \quad (\text{Eq. 44})$$

1) Liquid on Surface

$$g = \frac{2C_s \Delta t}{R_{nn}} \quad (\text{Eq. 45})$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn}} + a \right) \right] \Delta t \quad (\text{Eq. 46})$$

2) No Liquid on Surface

$$g = 0 \quad (\text{Eq. 47})$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn} + 2R_a} + a \right) \right] \Delta t \quad (\text{Eq. 48})$$

When there is only one outside slice which does not contain liquid the matrix system of Eq. 42 reduces to a single equation as follows:

$$B_{nn} m_{nn,j+1} = m_{nn,j} + gF + g \quad (\text{Eq. 49})$$

$$\text{where } gF = \frac{2C_s \Delta t}{R_{nn}} \quad (\text{Eq. 50})$$

$$\text{and } g = 0 \quad (\text{Eq. 51})$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn}} + \frac{2}{R_{nn} + 2R_{a2}} + a \right) \right] \Delta t \quad (\text{Eq. 52})$$

When there is no liquid at all in the clothing, the equations for vapour transport can be expressed by one matrix system as follows:

$$\begin{bmatrix} B_1 & C_2 & 0 & \dots & \dots & 0 \\ A_1 & B_2 & C_3 & 0 & \dots & \dots \\ 0 & A_2 & B_3 & B_4 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & A_{nn-1} & B_{nn-1} & C_{nn} \\ 0 & \dots & \dots & 0 & A_{nn-1} & B_{nn} \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nn,j+1} \end{bmatrix} = \begin{bmatrix} m_{1,j} \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \\ m_{nn,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ \dots \\ \dots \\ \dots \\ 0 \\ g \end{bmatrix} \quad (\text{Eq. 53})$$

where

$$A_1 = 0 \quad (\text{Eq. 54})$$

$$B_1 = 0 \quad (\text{Eq. 55})$$

$$gF = 0 \quad (\text{Eq. 56})$$

1) Liquid on Surface

$$g = \frac{2C_s \Delta t}{R_{nn}} \quad (\text{Eq. 57})$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn}} \right) + a \right] \Delta t \quad (\text{Eq. 58})$$

2) No Liquid on Surface

$$g = 0 \quad (\text{Eq. 59})$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}} \left(\frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn} + 2R_a} \right) + a \right] \Delta t \quad (\text{Eq. 60})$$

All three matrices given by Eq. 34, Eq. 42 and Eq. 53 are of the same form and can be written in matrix notation as follows:

$$\tilde{A} \vec{M}_{j+1} = \vec{M}_j + \vec{G} \quad (\text{Eq. 61})$$

where

\vec{M}_j is the mass of vapour per unit area in each slice of the system at a given point in time $j\Delta t$

\vec{M}_{j+1} is the vector of mass per unit area after the next time increment

\tilde{A} is the tridiagonal matrix of coefficients of the

absorptive and diffusive properties of the system

\vec{G} is the vector of boundary conditions

For a given set of initial conditions, the solution to the problem, which can readily be obtained by the Gauss elimination method (Westlake), is then:

$$\vec{M}_{j+1} = \tilde{A}^{-1} (\vec{M}_j + \vec{G}) \quad (\text{Eq. 62})$$

for the two matrices given by Eq. 34 and Eq. 42 when the clothing contains liquid and for the matrix of Eq. 53 when the clothing contains only vapour, except when only one outside slice does not contain liquid. Then the solution for this slice is:

$$m_{nn,j+1} = \frac{m_{nn,j} + gF}{B_{nn}} \quad (\text{Eq. 63})$$

4. AUXILIARY RELATIONSHIPS

a) Loss of Liquid

As vapour is transported away from liquid-vapour interfaces, the amount of liquid in the liquid containing slice must be reduced to balance it. In addition, there is a loss due to decomposition, which also occurs in internal slices within the clothing layers containing liquid. The liquid initially on the clothing surface is gradually lost due to evaporation to the air, and when the slice of clothing next to the surface contains no liquid, there is an additional loss due to vapour transport into the clothing.

The liquid losses were accounted for in each time step along with the vapour transport, previously described, as follows.

(1) First inside slice containing liquid

The first inside slice containing liquid is designated $nk + 1$ (Fig. 2). The loss of liquid from this slice was determined using the electrical analogy (Fig. 1) for vapour transport. Application of Kirchoff's law for flow into slice $nk + 1$ gives:

$$\frac{dm_{nk+1}}{dt} = \left(\frac{m_{nk}}{V_{nk}} - C_s \right) \frac{2}{R_{nk}} - aC_s V_{nk+1} \quad (\text{Eq. 64})$$

Discretizing for time step $j\Delta t$ to $(j+1)\Delta t$ then gives:

$$m_{nk+1,j+1} = m_{nk+1,j} + \frac{2m_{nk,j}\Delta t}{V_{nk}R_{nk}} - \frac{2C_s\Delta t}{R_{nk}} - aC_s V_{nk+1}\Delta t \quad (\text{Eq. 65})$$

There is a special case when the first inside slice containing liquid is adjacent to the skin. The value of R_{nk} is zero for the outer skin slice, which gives rise to terms of infinite value in Eq. 65. This was adjusted in the same manner as for vapour transport, described in section 3.b)(3). Thus, for slice $nk+1$, (Eq. 65) is replaced by the following equation:

$$m_{nk+1,j+1} = m_{nk+1,j} + \frac{2m_{nk,j}\Delta t}{V_{nk}R_{nk+1}} - \frac{2C_s\Delta t}{R_{nk+1}} - aC_s V_{nk+1}\Delta t \quad (\text{Eq. 66})$$

(2) First outside slice containing liquid

The first outside slice containing liquid is designated $nl-1$ (Fig. 2). Application of Kirchoff's law for flow into this slice gives:

$$\frac{dm_{nl-1}}{dt} = \left(\frac{m_{nl}}{V_{nl}} - C_s \right) \frac{2}{R_{nl}} - aC_s V_{nk+1} \quad (\text{Eq. 67})$$

Discretizing for time step $j\Delta t$ to $(j+1)\Delta t$ then gives:

$$m_{nl-1,j+1} = m_{nl-1,j} + \frac{2m_{nl,j}\Delta t}{V_{nl}R_{nl}} - \frac{2C_s\Delta t}{R_{nl}} - aC_s V_{nk+1}\Delta t \quad (\text{Eq. 68})$$

There is also a special case for the first outside slice containing liquid. This occurs at the outside slice of clothing, which is designated $i = nn$ (Fig. 2). When there is no liquid on the surface Kirchoff's law for flow into slice nn gives:

$$\frac{dm_{nn}}{dt} = - \frac{C_s\Delta t}{R_a} - aC_s V_{nn}\Delta t \quad (\text{Eq. 69})$$

Discretizing gives:

$$m_{nn,j+1} = m_{nn,j} - \frac{C_s \Delta t}{R_a} - a C_s V_{nn} \Delta t \quad (\text{Eq. 70})$$

When there is liquid on the surface, Eq. 70 reduces to:

$$m_{nn,j+1} = m_{nn,j} - a C_s V_{nn} \Delta t \quad (\text{Eq. 71})$$

(3) Middle slices

The middle slices in the clothing are designated i , where $nk + 1 < i < n\ell - 1$ (Fig. 2). Since the reduction of liquid in these slices is by decomposition only, Kirchoff's law for flow into one of these is:

$$\frac{dm_i}{dt} = -a C_s V_i \quad nk + 1 < i < n\ell - 1 \quad (\text{Eq. 72})$$

Discretizing gives:

$$m_{i,j+1} = m_{i,j} - a C_s V_i \Delta t \quad nk + 1 < i < n\ell - 1 \quad (\text{Eq. 73})$$

Note that the rate of loss by decomposition throughout the model is assumed to be $a C_s V_i$ whenever $m_i/V_i \geq C_s$. Also note that C_s is only used as a potential whenever $m_i/V_i \geq C_s$.

(4) Only one slice containing liquid

When there is only one slice in the clothing which contains liquid $nk + 1 = n\ell - 1$ (Fig. 2). The loss to the inside is given by Eq. 65 or Eq. 66, and the loss to the outside is given by one of Eq. 68, 70 or 71. However, in order not to apply the decomposition twice the quantity $a C_s V_{n\ell+1} \Delta t$ was added to the equation for the outside slice whenever $nk + 1 = n\ell - 1$.

(5) Loss of liquid from outside clothing surface

When there is no liquid in the outer slice of clothing, Kirchoff's law for the flow of vapour away from the liquid on the clothing

surface gives:

$$\frac{dQ}{dt} = \left(C_s - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn}} + \frac{C_s}{R_a} \quad (\text{Eq. 74})$$

where Q is the total amount of surface liquid lost to vapour evolution.

Discretizing gives:

$$Q_{j+1} = Q_j + \frac{2C_s \Delta t}{R_{nn}} - \frac{2m_{nn} \Delta t}{V_{nn} R_{nn}} + \frac{C_s \Delta t}{R_a} \quad (\text{Eq. 75})$$

When there is liquid in the outer slice of clothing Eq. 75 reduces to:

$$Q_{j+1} = Q_j + \frac{C_s \Delta t}{R_a} \quad (\text{Eq. 76})$$

b) Total Loss of Vapour to Air

The initial liquid on and in clothing is lost to air, to vapour in clothing, to the systemic sink and to decomposition. After the liquid is gone from the surface, there is a further vapour loss to air from the clothing. Now, if the vapour loss to air is accounted for, it is possible to calculate the loss due to decomposition, because this is the mass deficiency in the sums of the vapour and liquid in the total system. Alternatively, if the decomposition is set to zero, the calculation of vapour transport can be checked at each time step by observing that the total mass in the system must be constant.

The loss of vapour to air was accounted for in each time step as follows:

(1) No liquid in the outside clothing slice or on the surface

Application of Kirchoff's law using the electrical analogy (Fig. 1) for vapour transport to air from the outside clothing slice gives:

$$\frac{dU}{dt} = \frac{m_{nn}}{V_{nn}} \left(\frac{2}{R_{nn} + R_a} \right) \quad (\text{Eq. 77})$$

where U is the total vapour loss to air.

Discretizing gives:

$$U_{j+1} = U_j = \frac{2m_{nn}\Delta t}{V_{nn}(R_{nn} + 2R_a)} \quad (\text{Eq. 78})$$

(2) Liquid in the outside clothing slice or on the surface

Kirchoff's law gives: $\frac{dU}{dt} = \frac{C_s}{R_a}$ (Eq. 73)

Discretizing gives: $U_{j+1} = U_j + \frac{C_s \Delta t}{R_a}$ (Eq. 74)

c) Maximum Allowable Size of Time Increment

The chosen time increment for the calculation of vapour transport must be such that the mass in a slice never becomes negative, otherwise solutions become unstable. Experience has shown that this can occur for liquid reduction in slice $nk+1$ as calculated from Eq. 65 when the increment is too large. Analysis of Eq. 65 then provided a relationship for predetermining an approximate upper limit for the time step size. This was done in the following way:

For $m_{nk+1,j+1} \geq 0$ in Eq. 65 we must have:

$$\Delta t \left(\frac{2m_{nk,j}}{V_{nk}R_{nk}} - \frac{2C_s}{R_{nk}} - aC_s V_{nk+1} \right) \leq m_{nk+1,j} \quad (\text{Eq. 81})$$

Liquid must be present whenever Eq. 65 is used. Therefore:

$$m_{nk+1,j} \geq C_s V_{nk+1} \quad (\text{Eq. 82})$$

Substitution of Eq. 82 into Eq. 81 and rearranging gives:

$$\Delta t \leq \frac{C_s V_{nk+1}}{C_s \left(\frac{2}{R_{nk}} + aV_{nk+1} \right) - \frac{2m_{nk}}{V_{nk}R_{nk}}} \quad (\text{Eq. 83})$$

A simplified but slightly stronger restriction on the maximum

size of the time increment is obtained by setting the second term in the denominator of Eq. 83 to zero.

$$\text{Thus } \Delta t \leq \frac{R_{nk} V_{nk+1}}{2 + a R_{nk} V_{nk+1}} \quad (\text{Eq. 84})$$

5. COMPUTER PROGRAM

A computer program was written to solve the problem of vapour transport by means of the mathematical model described in the previous sections. A listing of the program along with one set of output results is shown in Appendix A. The listing is annotated in detail to describe the function of each part of the program and the input data required.

The program is written in the basic Fortran IV language of the DRES 1130 model 2C computer which has 16K words of core storage. The program in its present form requires approximately 9K of core storage. It will allow up to four layers of clothing to be simulated over skin with a total of fifty slices in the system. The skin is usually divided into seven slices, which leaves forty three slices for the clothing layers.

6. RESULTS

The computer program was applied to compare the systemic dose for various distributions of a 1.2 mg cm^{-2} initial load on and in two layers of clothing. The absorptive and diffusive properties used were chosen for test purposes only, and, in the author's knowledge, do not represent any real liquid and clothed skin system. The resistance, capacitance and saturated vapour concentration used are those shown in the sample computer output (Appendix A). The calculations were done for two different windspeeds to show the effect of varying windspeed on the total systemic dose for various load distributions. The results for five load distributions are shown in Table 1 and Table 2 for windspeeds of 6.87 cm sec^{-1} and 100 cm sec^{-1} respectively.

Also, using the same five initial load distributions, the pro-

gram was applied for 5, 10 and 20 slices in each of two layers and times of 1.0 and 0.1 minutes combined as shown in Table 3. The systemic dose and percentage of initial mass are also recorded in Table 3 to show the effect of varying the number of clothing slices and the time increment size on the results. In these tests, the decomposition was set to zero so that the total mass of agent should theoretically remain constant. The mass deficiency indicated in Table 3 is then only due to approximations caused by discretizing the skin clothing system.

7. DISCUSSION

The results shown in Table 1 and Table 2 indicate that the wind-speed over the clothing surface has a considerable effect on the systemic dose for all five loading configurations tested. The largest effect occurs when the initial load is placed at the surface, and the effect decreases as the initial load is distributed closer to the skin. Also, the systemic dose is increased as the initial load is distributed closer to the skin, as one would intuitively expect.

The results in Table 3 for various time step sizes and number of clothing slices indicate that, for practical purposes, even the most coarse discretization produces sufficient accuracy. Another method of discretization was tried for the slices at liquid-vapour interfaces. Instead of assuming that the diffusive resistance started exactly at the interface as was done in the present model, except for the skin-clothing interface, the assumed resistance included half that of the liquid containing slice. The difference in results between these two methods was found to be less than one percent, for the test data used to obtain the results in Table 1. Therefore, either method produces sufficiently accurate results for practical purposes.

8. CONCLUSIONS

A mathematical model and an associated computer program have been produced to calculate the systemic dose for an initial liquid loading on or

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/20

in the clothing of a clothed skin system. The program can be applied to practical problems for any liquid agent, when the diffusive and absorptive properties of a given system are known.

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The results shown in Table 1 and Table 2 indicate that the wind speed over the clothing surface has a considerable effect on the system dose for all five loading configurations tested. The largest effect occurs when the initial load is placed at the surface, and the effect decreases as the initial load is distributed closer to the skin. Also, the systemic dose is increased as the initial load is distributed closer to the skin, as one would intuitively expect.

The results in Table 3 for various time step sizes and number of clothing slices indicate that, for practical purposes, even the most coarse discretization produces sufficient accuracy. Another method of discretization was tried for the slices at liquid-vapor interfaces. Instead of assuming that the diffusive resistance started exactly at the interface as was done in the present model, except for the skin-clothing interface, the assumed resistance included half that of the liquid containing slice. The difference in results between these two methods was found to be less than one percent, for the test data used to obtain the results in Table 1. Therefore, either method produces sufficiently accurate results for practical purposes.

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A numerical test model and an associated computer program have been produced to calculate the systemic dose for an initial liquid loading on or

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TABLE 1

COMPARISON OF SYSTEMIC DOSES FOR VARIOUS
DISTRIBUTIONS OF 1.2 mg cm^{-2} LOADING AND
WINDSPEED OF 6.87 cm sec^{-1}

INPUT DATA						RESULTS
Loading mg cm^{-2}			Decay	MS	DELT	Systemic Dose
Surface	Top Layer	Bottom Layer	min^{-1}	No.	min	at 29 Hours mg cm^{-2}
1.2	0	0	0.003	20	0.1	0.01297
0.8	0.4	0	0.003	20	0.1	0.01359
0.4	0.8	0	0.003	20	0.1	0.01417
0	1.2	0	0.003	20	0.1	0.01473
0.4	0.4	0.4	0.003	20	0.1	0.01541

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TABLE 2

COMPARISON OF SYSTEMIC DOSES FOR VARIOUS
DISTRIBUTIONS OF 1.2 mg cm^{-2} LOADING AND
WINDSPEED OF 100 cm sec^{-1}

INPUT DATA						RESULTS
Loading mg cm^{-2}			Decay	MS	DELT	Systemic Dose
Surface	Top Layer	Bottom Layer	min^{-1}	No.	min	at 29 Hours mg cm^{-2}
1.2	0	0	0.003	20	0.1	0.00260
0.8	0.4	0	0.003	20	0.1	0.00345
0.4	0.8	0	0.003	20	0.1	0.00430
0	1.2	0	0.003	20	0.1	0.00516
0.4	0.4	0.4	0.003	20	0.1	0.00600

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TABLE 3

COMPARISON OF RESULTS FOR VARIOUS TIME STEP SIZES AND
NUMBER OF SLICES IN EACH CLOTHING LAYER

INPUT DATA						CALCULATED RESULTS FOR WINDSPEED 6.87 cm sec ⁻¹		
Loading mg cm ⁻²			Decay	MS	DELT	Results at 29 Hours mg cm ⁻²		
Surface	Top Layer	Bottom Layer	min ⁻¹	No.	min	Systemic Dose	Total Mass	% of Initial Mass
1.2	0	0	0	5	1.0	0.04734	1.1699	97.49
0.8	0.4	0	0	5	1.0	0.04948	1.1707	97.56
0.4	0.8	0	0	5	1.0	0.05056	1.1691	97.43
0	1.2	0	0	5	1.0	0.05150	1.1707	97.56
0.4	0.4	0.4	0	5	1.0	0.05323	1.1637	96.97
1.2	0	0	0	5	0.1	0.04796	1.1970	99.75
0.8	0.4	0	0	5	0.1	0.05029	1.1974	99.78
0.4	0.8	0	0	5	0.1	0.05129	1.1972	99.76
0	1.2	0	0	5	0.1	0.05206	1.1973	99.77
0.4	0.4	0.4	0	5	0.1	0.05409	1.1975	99.79
1.2	0	0	0	10	0.1	0.04790	1.1940	99.50
0.8	0.4	0	0	10	0.1	0.05013	1.1945	99.54
0.4	0.8	0	0	10	0.1	0.05125	1.1945	99.54
0	1.2	0	0	10	0.1	0.05207	1.1945	99.54
0.4	0.4	0.4	0	10	0.1	0.05413	1.1955	99.63
1.2	0	0	0	20	0.1	0.04777	1.1881	99.00
0.8	0.4	0	0	20	0.1	0.04995	1.1896	99.13
0.4	0.8	0	0	20	0.1	0.05108	1.1876	98.97
0	1.2	0	0	20	0.1	0.05196	1.1823	98.94
0.4	0.4	0.4	0	20	0.1	0.05367	1.1758	97.98

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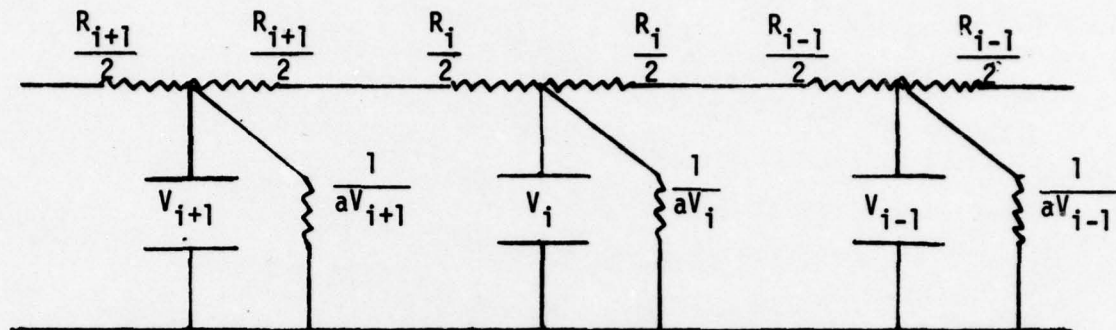


Figure 1: Analogous Electrical Network
for Non-Boundary Slices

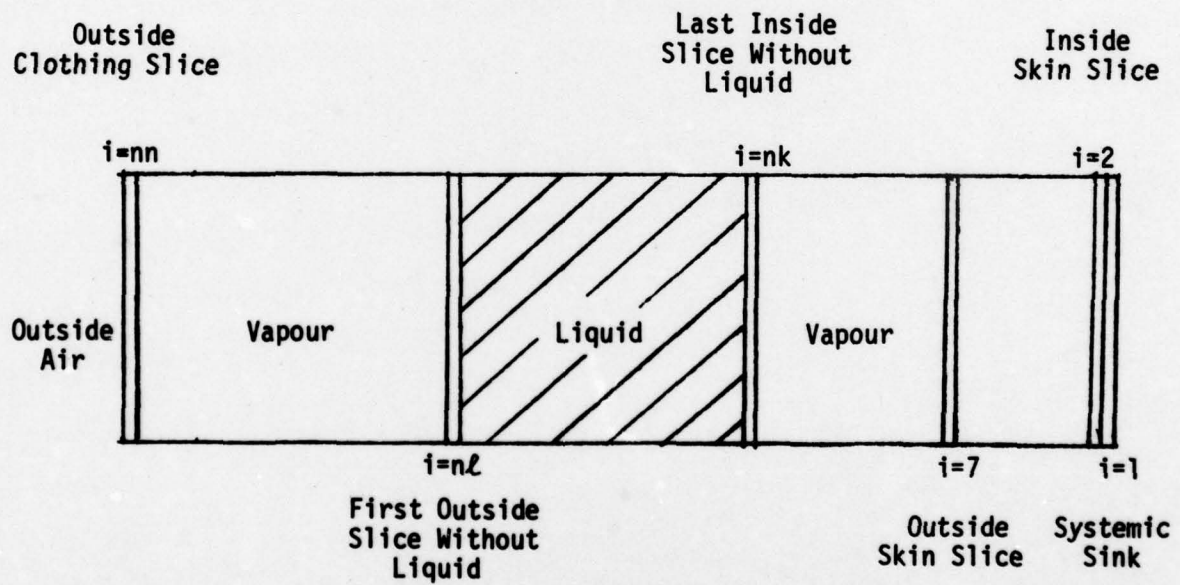


Figure 2: Clothed Skin System Showing Designation of
Boundary Slices

APPENDIX A

COMPUTER PROGRAM WITH RESULTS
FOR ONE SET OF DATA

```

PAGE 1
// JOB T
LOG DRIVE CART SPEC CART AVAIL PHY DRIVE
0000 0206 0206 0000
V2 M11 ACTUAL 16K CONFIG 16K
// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
SUBROUTINE AGENT(RTHIN,VTHIN,RAVEG,VAVEG,U,R,V,RA1,RA2,N,NS,DECAY,
1 INDEX)
C
C THIS SUBROUTINE CALCULATES THE RESISTANCE AND CAPACITANCE OF A
C SLICE OF THE TRANSITIONAL LAYER OF SKIN AND OF THE AIR.
C
C
C DIMENSION R(2),V(2),INDEX(5),A(80)
C WRITE(3,200)
C READ(2,100)(A(I),I=1,80)
C
C WRITE(3,201)
C WRITE (3,205) (A(I),I=1,80)
C GO TO (3,4),NS
3 R(2)=RAVEG/FLOAT(N-2)
V(2)=VAVEG/FLOAT(N-2)
WRITE(3,202) RAVEG,VAVEG
C GO TO 5
4 R(2) = RTHIN/FLOAT(N-2)
V(2) = VTHIN/FLOAT(N-2)
WRITE(3,203) RTHIN,VTHIN
5 RA1 = 0.9/U**0.78
RA2 = RA1
WRITE(3,204) U,RA1,DECAY
DO 6 I = 1,5
6 INDEX(I) = 0
C
C FORMATS FOR INPUT AND OUTPUT STATEMENTS
C
100 FORMAT(80A1)
200 FORMAT(11,33X,'A MATHEMATICAL MODEL FOR THE PENETRATION')
201 FORMAT(48X,'OF CLOTHING AND SKIN')
202 FORMAT(11,42X,'SKIN TYPE - AVERAGE',/44X,'RESISTANCE =',F7.3,3X,
1 'THIN/CM',/44X,'CAPACITANCE =',F7.1,3X,'(CM)')
203 FORMAT(11,42X,'SKIN TYPE - THIN',/44X,'RESISTANCE =',F7.3,3X,'(M
1IN/CM',/44X,'CAPACITANCE =',F7.1,3X,'(CM)')

```


PAGE 2

204 FORMAT(,42X,'WINDSPEED = ',F6.2,6X,'(CM/SEC)',/,42X,'BOUNDARY LAY
ER RESISTANCE',F9.3,2X,'(MIN/CM)',/,42X,'DECOMPOSITION RATE',10X,F
25.3, 2X,'(1/MIN)')
205 FORMAT(,20X,80A1,/))

RETURN
END

VARIABLE ALLOCATIONS
AIR 1=00FD-0000 III 1=00F3

STATEMENT ALLOCATIONS

100 =0102 200 =0105 201 =011E 202 =0128 203 =015A 204 =0187 205 =01C3 3 =022D 4 =0255 5 =0278
6 =0296

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SURPROGRAMS
FAXR ELD ESTO ESTOX EDVR FLOAT SRED SWRT SCOMP SIOFX SIOF SUBSC SUBIN

REAL CONSTANTS
.900000000E 00=00F6 .780000000E 00=00F9

INTEGER CONSTANTS
1=00FC 2=00FD 1=00FE 80=00FF 5=0100 0=0101

CORF REQUIREMENTS FOR AGENT
COMMON 0 VARIABLES 246 PROGRAM 436

RELATIVE ENTRY POINT ADDRESS IS 01C9 (HEX)

END OF COMPILATION

// DUP

*STORE WS UA AGENT
CART ID 0206 DB ADDR 4020 DB CNT 001C

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SURROUTINE INDX(DELTA,TOTAL,TN,TD,TR,TOTL,NTN,NTD,NTR)
C THIS SURROUTINE CHANGES THE VARIOUS INPUT TIMES TO INTEGER FORM.
C

PAGE 3

```
NTOTL = IFIX(TOTAL*60.0/DELT + 0.00001)
NTN = IFIX(TN*60.0/DELT + 0.00001)
NTD = IFIX(TD*60.0/DELT + 0.00001)
NTR = IFIX(TR*60.0/DELT + 0.00001)
WRITE(3,200) TOTAL,TD,TN,DELT
200 FORMAT(//,4X,'TIME CONSTANTS',/,4X,'TOTAL TIME',8X,'=',F7.2,3X,'
1(HOURS)',/,4X,'TIME OF DECONTAM =',F7.2,3X,'(HOURS)',/,4X,'TIME
2 INCREMENT =',F7.2,3X,'(HOURS)',/,4X,'DELT =',F6.3,3X,'(MINU
3TES)',/,///)
```

C RETURN
END

STATEMENT ALLOCATIONS
200 =000E

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS
EADD EMPY EDIV ELD ESTO IFIX SWRT SCOMP SIOF SUBIN

REAL CONSTANTS
.600000000E 02=0004 .100000000E-04=0007

INTEGER CONSTANTS
3=000A

CORE REQUIREMENTS FOR INDXX
COMMON 0 VARIABLES 4 PROGRAM 198

RELATIVE ENTRY POINT ADDRESS IS 0063 (HEX)

END OF COMPILATION

// DUP

*STORE WS UA INDXX
CART ID 0206 DB ADDR 4D3C DB CNT 000E

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
SUBROUTINE CONST(N,N,NUM,NK,DELT,DECAY,RA1,RA2,R,V,RT,VT,MS,A,B,C

PAGE 4

1)

THIS SUBROUTINE CALCULATES THE RESISTANCE AND CAPACITANCE OF EACH SLICE OF CLOTHING AND SKIN AND ALSO CALCULATES THE COMPONENTS OF THE MATRIX OF COEFFICIENTS.

DIMENSION V(50),R(50),VT(5),RT(5),MS(4),A(50),B(50),C(50)

SKIN LAYERS

R(1) = 0.0

NK=N-1

DO 10 I=3,NK

V(I)=V(2)

10 R(I) = R(2)

MORNY LAYER

V(N)=5.*V(2)

R(N) = 0.0

CLOTH LAYERS

NK=N+1

DO 16 J=1,NUM

M1 = MS(J) + NK - 1

DO 13 I=NK,M1

R(I)=RT(J)/FLOAT(MS(J))

13 V(I)=VT(J)/FLOAT(MS(J))

16 NK = M1 + 1

OUTSIDE SLICE OF OUTER LAYER

NN = M1

NK=NN

SURFACE

R(NN+1) = RA2

TRIDIAGONAL MATRIX OF COEFFICIENTS IN DIFFERENTIAL EQUATIONS OF MASS TRANSPORT

B(1)=1.0

A(2)=0.0

R(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/(R(NK))/V(NK))+DECAY)

PAGE 5

```
DO 25 I=2,NK
  C(I-1) = -DELT*2.0/(V(I)*(R(I-1)+R(I)))
  IF(I-NK) 24,25,25
  24 A(I+1) = -DELT*2.0/(V(I)*(R(I)+R(I+1)))
  R(I) = 1.0 + DELT*(2.0/(R(I-1)+R(I))+2.0/(R(I) + R(I+1)))
  1/V(I) + DECAY)
  25 CONTINUE
```

C
RETURN
END

VARIABLE ALLOCATIONS
I(I) 1=0003 J(I) 1=0004 M(I) 1=0005

STATEMENT ALLOCATIONS
10 =0009 13 =00EB 16 =010B 24 =0186 25 =01CC

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS
EADD EADDX EMPY EMPYX EDIVX ELD ELDX ESTO ESTOX EDVR EDVRX FLOAT SUBSC SNR SUBIN

REAL CONSTANTS
.00C000000E 00=000C .500000000E 01=000F. .100000000E 01=0012 .200000000E 01=0015

INTEGER CONSTANTS
1=0018 3=0C19 2=001A

CORE REQUIREMENTS FOR CONST
COMMON 0 VARIABLES 12 PROGRAM 460

RELATIVE ENTRY POINT ADDRESS IS 001B (HEX)

END OF COMPILATION

// DUP

*STORE WS UA CONST
CARD ID 0206 DB ADDR 404A DB CNT 0020

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SUBROUTINE CLOTH(N,NN,NUM,NTIME,NTR,NK,INDEX,ITHLY,KTHSL,M,

PAGE 6

```

1R,B,G,U,DELT,RA2,DECAY,MASS,CS,MS,V,KIN,A,C,LIN,LTHLY,NL,LTHSL,
2NSURF,Q)
C
C THIS SUBROUTINE DETERMINES WHEN THE LIQUID IS GONE IN SUCCESSIVE
C SLICES AND CHANGES THE APPROPRIATE CONSTANTS
C AT LIQUID-VAPOR INTERFACES.
C
REAL M(50),MASS(5)
DIMENSION INDEX(5),R(50),B(50),MS(4),V(50),A(50),C(50)
IF(INDEX(1))1,1,2
C
C SET INITIAL CONDITIONS
C
1 CALL LIOPC(CS,NUM,N,MS,M,ITHLY,KTHSL,KIN,INDEX,
1LIN,LTHLY,U,NL,LTHSL,NSURF,Q,MASS)
2 IF(INDEX(1))3,3,310
C
C REPLACE CLOTHING AT DESIGNATED TIME
C
3 IF(INTR -NTIME)310,4,310
4 CALL CLREN(NTIME,N,NN,M,DELT,NK,INDEX,MASS,NSURF)
C
C CHECK FOR LIQUID ON SURFACE
C
310 IF(INDEX(5))5,5,10
5 IF(M(NN)-CS*V(NN))6,6,7
6 Q = 0 + DELT*(CS*(R(NN)+2.0*RA2)/(R(NN)*RA2) - M(NN)/(V(NN)*R(NN))/
12.0))
GO TO 8
7 Q=Q+DELT*CS/RA2
8 IF(Q-MASS(NSURF))10,9,9
9 IF(NTIME-1)312,312,311
311 TIME = FLOAT(NTIME)*DELT/60.0
WRITE(3,202)TIME
312 R(NN) = 1.0 + DELT*((2.0/(R(NN)-1)+R(NN)) + 2.0/(R(NN) +
12.0*RA2))/V(NN)+ DECAY)
C
C SET INDEX FOR LIQUID ALL GONE FROM SURFACE
C
INDEX(5)=INDEX(5)+1
C
C IF LIQUID ALL GONE IN CLOTHING USE TRID ACCORDINGLY
C
10 IF(INDEX(2)) 11,11,60
C
C FIND INNERMOST SLICE WHICH STILL CONTAINS LIQUID

```

PAGE 7

```
C
11 IF(M(KTHSL)-CS*(KTHSL)) 12,12,15
12 KTHSL=KTHSL+1
13 IF(KTHSL-NL)13,14,14
13 GO TO 11
C
C SET INDEX FOR LIQUID ALL GONE
C
14 INDEX(2)=INDEX(2) + 1
KTHSL=KTHSL-1
TIME=FLOAT(INTIME)*DEL/60.0
WRITE (3,201) TIME
IF(INDEX(4))1314,314,60
314 CONTINUE
WRITE(3,204)KTHSL
GO TO 60
C
C FIND OUTERMOST SLICE WHICH STILL CONTAINS LIQUID
C
15 IF(M(LTHSL) - CS*(LTHSL))16,16,26
16 LTHSL = LTHSL - 1
GO TO 11
C
C RECORD TIME AT WHICH LIQUID IS GONE FROM EACH SUCCESSIVE LAYER
C
26 IF((KTHSL-KIN)-MS(IHLY)) 28,27,27
27 TIME=FLOAT(INTIME)*DEL/60.0
WRITE(3,200) IHLY,TIME
KIN=KIN+ MS(IHLY)
IHLY=IHLY + 1
GO TO 26
28 IF((LIN-LTHSL)-MS(LHLY))30,29,29
29 TIME=FLOAT(INTIME)*DEL/60.0
WRITE(3,200)IHLY,TIME
LIN=LIN-MS(LHLY)
LHLY=LHLY-1
GO TO 28
C
C FIRST OUTER SLICE WHICH CONTAINS NO LIQUID
C
30 NL = LTHSL + 1
C
C VAPOUR TRANSPORT IN INNER SLICES
C
C SET NUMBER OF EQUATIONS IN TRID TO OUTER SLICE OF INSIDE SLICES
C CONTAINING NO LIQUID
```

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```
C
C
C      NK=KTHSL-1
C      NJ = 1
C      GF = 0.0
C
C      SPECIAL CASE OF LIQUID IN SLICE NEXT TO SKIN
C
C      IF(NK-N)35,34,35
C      34 G = 2.0 * DELT*CS/R(N+1)
C      M(N+1) = M(N+1) - DELT*(CS*(2./R(N+1)) + DECAY*V(N+1)) -M(N)/
C      1(V(N)*R(N+1)/2.0))
C      GO TO 36
C      35 G = 2.0 * DELT*CS/R(NK)
C
C      REDUCE MASS OF LIQUID IN INNER SLICE
C
C      W(NK+1) = M(NK+1) - DELT*(CS*(2./R(NK)) +DECAY*V(NK+1))- M(NK)/
C      1(V(NK)*R(NK)/2.0))
C      B(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/R(NK))/V(NK)+DECAY)
C      36 CALL TRIDIM(A,B,C,NK,G,NJ,GF)
C      B(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/(R(NK) + R(NK+1))))/
C      1V(NK)+ DECAY)
C
C      VAPOUR TRANSPORT IN OUTER SLICES
C
C      NK = NN
C      IF(Q-MASS(INSURF))141,42,42
C      41 G = 2.0*DELT*CS/R(NN)
C      GO TO 43
C      42 G = 0.0
C
C      SFT STARTING POINT OF TRID TO FIRST OUTER SLICE CONTAINING NO
C      LIQUID
C      43 NJ=NL
C      GF = 2.0*DELT*CS/R(NL)
C
C      REDUCE MASS OF LIQUID IN OUTER SLICE
C
C      IF(KTHSL - LTHSL)344,44,344
C      44 TEMP = DECAY
C      DECAY = 0.0
C      344 IF(NL-(NN+1))52,45,45
C      45 IF(Q-MASS(INSURF))146,49,49
C      46 M(NN)=M(NN)-DELT*DECAY*CS*V(NN)
C      U=U+DELT*CS/RA2
```


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```

GO TO 56
49 M(NN) = M(NN) - DELT*CS*1./RA2 + DECAY*V(NN)
U = U + DELT*CS/RA2
GO TO 56
52 IF(NL = NN) 54,53,53
53 M(NN-1) = M(NN-1) - DELT*(CS*(2./R(NN)) + DECAY*V(NN-1)) - M(NN)/
1(V(NN)*R(NN)/2.0)
IF(KTHSL = LTHSL)346,345,346
345 DECAY = TEMP
346 U = U + DELT*M(NN)/(V(NN)*R(NN)/2.0 + RA2)
R(NN) = 1.C + DELT*((2.0/R(NN)) + 2.0/(R(NN) +
12.0*RA2))/V(NN) + DECAY
C
C
C
SOLVE EQUATION FOR ONE SLICE INSTEAD OF CALLING TRID
M(NN) = (M(NN) + GF)/R(NN)
R(NN) = 1.0 + DELT*((2.0/R(NN-1)+R(NN)) + 2.0/R(NN) +
12.0*RA2))/V(NN) + DECAY
GO TO 356
54 M(NL-1) = M(NL-1) - DELT*(CS*(2./R(NL)) + DECAY*V(NL-1)) - M(NL)/
1(V(NL)*R(NL)/2.0)
IF(KTHSL = LTHSL)351,350,351
350 DECAY = TEMP
351 U = U + DELT*M(NN)/(V(NN)*R(NN)/2.0 + RA2)
R(NJ) = 1.0 + DELT*((2.0/R(NJ) + 2.0/R(NJ) + R(NJ+1))
1/V(NJ) + DECAY)
C
C
C
SOLVE EQUATIONS FOR TWO OR MORE SLICES
CALL TRID(M,A,B,C,NK,G,NJ,GF)
R(NJ) = 1.0 + DELT*((2.0/R(NJ-1) + R(NJ)) + 2.0/R(NJ) +
1R(NJ+1))/V(NJ) + DECAY
GO TO 356
C
C
C
REDUCE LIQUID MASS IN MIDDLE SLICES BY DECOMPOSITION ONLY
56 IF(KTHSL = LTHSL)356,355,356
355 DECAY = TEMP
356 L = KTHSL + 2
IF(L-LTHSL)57,57,99
57 CONTINUE
DO 58 I = L,LTHSL
58 M(I-1) = M(I-1) - DELT*DECAY*CS*V(I-1)
GO TO 99
C
C
C
LIQUID ALL GONE IN CLOTHING

```


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CORE REQUIREMENTS FOR CLOTH
COMMON 0 VARIABLES 22 PROGRAM 1810

RELATIVE ENTRY POINT ADDRESS IS 0092 (HEX)

END OF COMPILE

// DUP

*STORE WS UA CLOTH
CART ID 0206 DB ADDR 4D6A DB CNT 007E

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION

*LIST ALL

SUBROUTINE LIQPC(CS,NUM,N,MS,M,ITHLY,KTHSL,KIN,INDEX,
1LIN,LTHLY,U,NL,LTHSL,NSURF,Q,MASS)

THIS SUBROUTINE SETS THE INITIAL CONDITIONS.

REAL M(50),MASS(5)
DIMENSION MS(4),INDEX(5)

INPUT SATURATED VAPOR CONCENTRATION AND MASS OF LIQUID IN EACH
LAYER

NSURF=NUM+1
READ(2,100) CS,(MASS(I),I=1,NSURF)
WRITE(3,200) CS,(I,MASS(I),I=1,NUM)
WRITE(3,201)MASS(NSURF)
DO 30 I=1,NUM
IF(MASS(I)) 30,30,31

30 CONTINUE

INDEX FIRST LAYER CONTAINING LIQUID

31 ITHLY=I

INDEX INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID

KTHSL=N+1

IF(ITHLY-1) 32,32,33

33 DO 34 I=2,ITHLY

PAGE 12

C INDEX INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID

C 34 KTHSL=KTHSL + MS(I-1)

C SET INDEX OF INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID

C 12 KIN=KTHSL

C SET MASS EQUAL ZERO IN EACH LAYER WHICH CONTAINS NO LIQUID

C DO 35 I=2,KTHSL

C 35 M(I-1)=C.O

C INDEX SLICE AT BEGINNING OF FIRST LAYER WHICH CONTAINS LIQUID

C NN=KTHSL

C SET INDEX IF NO LIQUID IN CLOTHING

C IF(ITHLY-NUM)30,39,38

C 38 INDEX(2) = INDEX(2) + 1

C GO TO 40

C 39 CONTINUE

C INDEX OUTSIDE SLICE OF EACH LAYER IN TURN

C DO 36 J=ITHLY,NUM

C NK=MS(J)+NN-1

C SFT MASS IN EACH SLICE OF LAYERS WHICH CONTAIN LIQUID

C DO 37 L=NN,NK

C 37 M(L)=MASS(J)/FLOAT(MS(J))

C INDEX SLICE AT BEGINNING OF NEXT LAYER

C 36 NN=NK+1

C SFT INDICES AT OUTSIDE BOUNDARY

C LIN = NN-1

C LTHLY = NUM

C LTHSL = NN-1

C NL = NN

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C MASS LOSS TO ATMOSPHERE

C 40 U=0.0
0=0.0

C INITIAL CONDITIONS HAVE BEEN SET

C INDEX(1)=INDEX(1) + 1

C FORMATS FOR OUTPUT STATEMENTS

100 FORMAT(8F10.0)
200 FORMAT(//.42X,'SATURATED VAPOR CONCENTRATION', / ,58X,'SVC ='E11.4
1.2X,'(MG/CM**3)',//.49X,'INITIAL LIQUID LOADING',//,
2.42X,'MASS IN LAYER ',1.7X,F7.3,' MG/CM**2')
201 FORMAT(//.42X,'MASS ON SURFACE',8X,F7.3,' MG/CM**2')
RETURN

END

VARIABLE ALLOCATIONS

III)=0000 NM(I)=0001 J(I)=0002 NK(I)=0003 L(I)=0004

STATEMENT ALLOCATIONS

100 =000E 200 =0011 201 =0096 30 =00FD 31 =0106 33 =0116 34 =011A 32 =012E 35 =0136 38 =0152
39 =015C 37 =0171 36 =019B 40 =018E

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS

ELD ELDX ESTO ESTOX EDVRX FLOAT SRED SMRT SCOMP SIOFX SIOF SIOI SUBSC SUBIN

REAL CONSTANTS

.000000000E 00=0008

INTEGER CONSTANTS

1=0008 2=000C 3=000D

CORE REQUIREMENTS FOR LTOPC

COMMON 0 VARIABLES 8 PROGRAM 456

RELATIVE ENTRY POINT ADDRESS IS 0068 (HEX)

END OF COMPILATION

PAGE 14

// DUP

*STORE WS UA LTQPC
CART ID 0206 DB ADDR 4DE8 DB CNT 0010

// FOR

*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SUBROUTINE CLREM(NTIME,N,NN,M,DELT,NK,INDEX,MASS,NSURF)

C THIS SUBROUTINE SETS THE MASS OF AGENT ON AND IN CLOTHING TO
C ZFRO AT TIME OF CLOTHING REPLACEMENT.

REAL M(50),MASS(5)
DIMENSION INDEX(5)
K = N+1

TIME = FLOAT(NTIME)*DELT/60.0
WRITE(3,200) TIME

DO 2 I = K,NN

M(I) = 0.0

MASS(NSURF) = 0.0

INDEX(4) = INDEX(4) + 1

C FORMAT FOR OUTPUT STATEMENT

C

200 FORMAT(//,22X,'CLOTHING REPLACED AT T=',F6.2,2X,'(HOURS)',//)

RETURN

END

VARIABLE ALLOCATIONS
TIME(R 1=0000 K(I) =0003 I(I) =0004

STATEMENT ALLOCATIONS
200 =0010 2 =0056

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS
EMPY FDIV ELD

REAL CONSTANTS
.600000000E 02=C008 .000000000F 00=0000

INTEGER CONSTANTS
1=0000 3=000F

ESTO ESTOX FLOAT SWRT SCOMP SIOF SUBSC SUBIN

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CORE REQUIREMENTS FOR CLREM
COMMON 0 VARIABLES 8 PROGRAM 116

RELATIVE ENTRY POINT ADDRESS IS 0028 (HEX)

END OF COMPILATION

// DUP

*STORE WS UA CLREM
CART ID 0206 DB ADDR 4E05 DB CNT 0009

// FOR

*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SUBROUTINE DECON(TIME,MASS,NSURF,Q,EFFIC,DELT)

C THIS SUBROUTINE REDUCES THE MASS ON THE OUTER CLOTHING SURFACE
C AT THE TIME OF DECONTAMINATION.

REAL MASS(5)
TIME = FLOAT(TIME)*DELT/60.0
WRITE(3,200)TIME
Q = Q + EFFIC*MASS(NSURF)
MASS(NSURF) = (1.0 - EFFIC)*MASS(NSURF)

C FORMAT FOR OUTPUT STATEMENT

200 FORMAT(/,42X,'DECONTAMINATION AT T=',F6.2,2X,'(HOURS)',/)

C RETURN
END

VARIABLE ALLOCATIONS
TIME(R 1)=0000

STATEMENT ALLOCATIONS
200 =000R

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS
EADD FSUB EMPY

ESTO ESTOX FLOAT SWRT SCOMP SIOF SUBSC SUBIN

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REAL CONSTANTS
*600000000E 02=0004 *100000000E 01=0007

INTEGER CONSTANTS
3=000A

CORP REQUIREMENTS FOR DECON
COMMON 0 VARIABLES 4 PROGRAM 90

RELATIVE ENTRY POINT ADDRESS IS 0022 (HEX)

END OF COMPILATION

// DUP

*STORE WS UA DECON
CART ID 0206 DB ADDR 4E0E DB CNT 0007

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SUBROUTINE TRID(M,A,B,C,NK,GG,NJ,GF)

C THIS SUBROUTINE CALCULATES THE MASS OF VAPOUR IN EACH LAYER AS A
C FUNCTION OF TIME BY SOLUTION OF THE EQUATIONS OF MASS TRANSFER.
C GAUSSIAN ELIMINATION IS USED TO GET THE SOLUTION VECTOR FROM THE
C MATRIX OF COEFFICIENTS.

C REAL M(50)
C DIMENSION A(50),B(50),C(50),Q(200),W(200),G(200)

C VAPOUR IN OUTSIDE SLICE

C M(NK) = M(NK) + GG

C COEFFICIENT FOR INSIDE SLICE

C M(NJ) = M(NJ) + GF

C W(NJ) = B(NJ)

C G(NJ) = M(NJ)/W(NJ)

C REDUCTION TO TRIANGULAR FORM

C

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C THE NEW VALUES OF A ARE ZERO
C THE NEW VALUES OF B ARE ONE
C Q IS THE NEW VALUE OF C
C G IS THE NEW VALUE OF D
C D IS THE VALUE OF M INITIALLY
C

JJ = NJ + 1
DO 1 I=JJ,NK
Q(I-1) = C(I-1)/W(I-1)
W(I) = B(I)-A(I)*Q(I-1)
1 G(I) = (M(I) - A(I)*G(I-1))/W(I)

C BACK SUBSTITUTION TO OBTAIN SOLUTION VECTOR
C

JJ = NK-NJ+1
M(NK) = G(NK)
DO 2 I = 2,JJ
K = NK + 1 - I
2 M(K) = G(K) - Q(K)*M(K+1)

C RETURN
END

VARIABLE ALLOCATIONS
G(R) 1=0255-0000 W(R) 1=04AD-0250 G(R) 1=0705-0480 JJ(I) 1=0708 I(I) 1=0709 K(I) 1=070A

STATEMENT ALLOCATIONS
1 =077D 2 =0789

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS
EADD EMPYX EDIVX ELDX ESTOX ESBX SUBSC SUBIN

INTEGER CONSTANTS
1=070E 2=070F

CORE REQUIREMENTS FOR TRID
COMMON 0 VARIABLES 1806 PROGRAM 200

RELATIVE ENTRY POINT ADDRESS IS 0710 (HEX)

END OF COMPILATION

BYOB 19

PAGE 18

// DUP

*STORE MS UA TRID
CART ID 0206 DB ADDR 4E15 DB CNT 000F

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL

SUBROUTINE PROUT(NUM,N,NTIME,M,MS,U,DELT,INDEX)

C THIS SUBROUTINE PRINTS THE CALCULATED MASS OF AGENT IN EACH
C LAYER AS A FUNCTION OF TIME.

REAL M(50)
DIMENSION INDEX(5),SUM(5),MS(4)

C TIME=FLOAT(NTIME)*DELT/60.0 + 0.00001

DO 20 I=1,5

20 SUM(I)=C.0

C IF(INDEX(3)) 21,21,40

21 WRITE(3,200)

INDEX(3)=INDEX(3) + 1

IF(NUM=4) 27,27,28

27 NM=NUM

GO TO 29

28 NM=4

29 GO TO (30,31,32,33),NM

30 WRITE(3,201)

GO TO 40

31 WRITE(3,202)

GO TO 40

32 WRITE(3,203)

GO TO 40

33 WRITE(3,204)

40 DO 47 I=3,N

47 SUM(I)=SUM(I) + M(I-1)

K=N+1

KNK=NM + 1

DO 55 J=2,KNK

KK=K-1+MS(J-1)

DN 56 I=K,KK

56 SUM(J)=SUM(J) + M(I)

55 K=KK+1

C

C FORMATS FOR OUTPUT STATEMENTS

```

WRITE(3,205)TIME,U,M(1),SUM(1),M(N),SUM(1),I=2,KNK)
200 FORMAT(11,44X,'MASS IN EACH LAYER IN MG/CM**2',/)
201 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
1,'MASS IN',/,'1X','HOURS',1X,'MG/CM**2',4X,'DOSE',9X,'TRANSITIONAL',
26X,'HORNY',7X,'FIRST CLOTH',/,'35X',3('LAYER',10X),/)
202 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
1,'MASS IN',8X,'MASS IN',/,'1X','HOURS',1X,'MG/CM**2',4X,'DOSE',9X,'T
2TRANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',4X,'SECOND CLOTH',/,'35X',4
3('LAYER',10X),/)
203 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
1,'MASS IN',8X,'MASS IN',8X,'MASS IN',/,'1X','HOURS',1X,'MG/CM**2',4X
2,'DOSE',9X,'TRANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',4X,'SECOND C
3LOTH',9X,'THIRD CLOTH',/,'35X',5('LAYER',10X),/)
204 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
1,'MASS IN',8X,'MASS IN',8X,'MASS IN',8X,'MASS IN',/,'1X','HOURS',1X,
2MG/CM**2',4X,'DOSE',9X,'TRANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',
34X,'SECOND CLOTH',3X,'THIRD CLOTH',4X,'FOURTH CLOTH',/,'35X',5('LAYE
4R',10X),,'LAYER',/)
205 FORMAT(7.3,F8.5,7(2X,F10.7,3X))

```

RETURN

END

VARIABLE ALLOCATIONS

```

SUM(I)=000C-0000 TIME(I)=000F
J(I)=0016 KK(I)=0017

```

KNK(I)=0015

K(I)=0014

NM(I)=0013

I(I)=0012

TIME(I)=000F

J(I)=0016

KK(I)=0017

STATEMENT ALLOCATIONS

```

200 =002A 201 =0040 202 =008F 203 =00EC 204 =0157 205 =01D4 20 =0206 21 =021E 27 =0230 28 =0236
29 =023A 30 =0242 31 =0248 32 =024E 33 =0254 40 =0258 47 =025C 56 =0297 55 =0286

```

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION

CALLED SUBPROGRAMS

```

EADD EADDX EMPY EDIV ELD ELDX ESTO ESTOX FLOAT SWRT SCOMP SIOF SUBSC SUBIN

```

REAL CONSTANTS

```

.400000000F 02=001C .100C000000E-04=001F .000000000E 00=0022

```

INTEGER CONSTANTS

```

1=0025 5=0026 3=0027 4=0028 2=0029

```

CORE REQUIREMENTS FOR PROUT

```

COMMON 0 VARIABLES 28 PROGRAM 724

```

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RELATIVE ENTRY POINT ADDRESS IS 01DC (HEX)

END OF COMPILATION

// DUP

*STORE NS UA PROUT
CARD ID 0206 DB ADDR 4E24 DB CNT 002C

// FOR

*ONE WORD INTEGERS
* EXTENDED PRECISION
* IOC(SICARD)
* IOC(SI132 PRINTER)
* IOC(SIDISK)
* LIST ALL

INPUT DATA FOR LIQUID ON AND IN CLOTH PROGRAM

CARD 1 - 213

NAME

N - TOTAL NUMBER OF SLICES SKIN IS DIVIDED INTO

NS=1 AVERAGE SKIN

NS=2 THIN SKIN

CARD 2 - 8F10.3

RTHIN,VTHIN,RAVEG,VAVEG,U,DECAY,DELT,EFFIC

RTHIN,RAVEG - RESISTANCE OF SKIN TYPES (MIN/CM)

VTHIN,VAVEG - CAPACITANCE OF SKIN TYPES (CM)

U - WIND SPEED (CM/SEC)

DECAY - DECAY FACTOR (PER CENT*10**2 PER MINUTE)

DELT - TIME INCREMENT IN MINUTES

EFFIC - EFFICIENCY OF DECONTAMINATION

CARD 3 - 8F10.3

TOTAL,TN,TD,TR

TOTAL - TOTAL TIME PERIOD (HOURS)

TN - TYPE OUT INCREMENT (HOURS)

TD - TIME OF DECONTAMINATION (HOURS)

TR - TIME OF REMOVAL OF CLOTHING (IF APPLICABLE),(HOURS)

CARD 4 - 80A1 (IN SUBROUTINE AGENT)

A(I)

A(I) - IDENTIFICATION OF AGENT AND APPLICATION

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```

C CARD 5 - 13
C NUM
C NUM - NUMBER OF LAYERS OF CLOTHING. THE PROGRAM WILL ACCEPT
C ANY NUMBER OF LAYERS BUT ONLY THE CONTENTS OF THE INNERMOST 4
C WILL BE PRINTED. FOR MORE THAN 5 LAYERS, THE DIMENSION
C STATEMENTS MUST BE ALTERED.
C
C CARD 6A - 13,2F10.0
C MS(1),RT(1),VT(1)
C ONE CARD PER CLOTHING LAYER (STARTING WITH THE INNERMOST)
C MS - NUMBER OF SLICES THAT EACH LAYER IS SUBDIVIDED INTO
C RT - RESISTANCE OF EACH LAYER (MIN/CM)
C VT - CAPACITANCE OF EACH LAYER (CM)
C
C CARD 7 - 8F10.0 (IN SUBROUTINE LIOPC)
C CS,MASS(1)
C CS - SATURATED VAPOUR CONCENTRATION (MG/CM**3)
C MASS(1) - MASS IN CLOTHING AT T=0 (MG/CM**2) I=1,NUM
C AND ON CLOTHING I=NUM+1
C
C CARD 8 - 213
C START OF ANOTHER SET OF DATA OR CALL EXIT
C N - CALLS EXIT IF ZERO OR NEGATIVE
C
C REAL M(50), MASS(5)
C DIMENSION A(50),B(50),C(50),R(50),V(50),RT(5),VT(5),MS(4),INDEX(5)
C
C 1 READ(2,100) N,NS
C IF(N)99,99,2
C
C 2 READ(2,101) RTHIN,VTHIN,RAVEG,VAVEG,U,R,V,RA1,RA2,N,NS,DECAY,INDEX
C READ(2,101) TOTAL,TN,TD,TR
C CALL AGENT(RTHIN,VTHIN,RAVEG,VAVEG,U,R,V,RA1,RA2,N,NS,DECAY,INDEX)
C DO 3 I=1,4
C 3 MS(I) = 0
C READ(2,102)NUM,(MS(1),RT(1),VT(1),I=1,NUM)
C WRITE(3,200)
C WRITE(3,201) (I,MS(1),RT(1),VT(1),I=1,NUM)
C
C CALL INDXX(DELTA,TOTAL,TN,TD,TR,NTOTL,NTN,NTD,NTRI)
C CALL CONST(N,NN,NUM,NK,DELTA,DECAY,RA1,RA2,R,V,RT,VT,MS,A,B,C)
C
C NTT = NTN
C
C NTIME = 1
C

```

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```

14 CALL CLOTHIN,N,N,NUM,NTIME,NTR,NK,INDEX,ITHLY,KTHSL,M,R,B,G,
15 DELT,RAZ,DECAY,MASS,CS,MS,V,KIN,A,C,LIN,LTHLY,NL,LTHSL,NSURF,Q)
16 IF(NTIME - NTD)17,16,17
16 CALL DECON(NTIME,MASS,NSURF,Q,EFFIC,DELT)
17 IF(NTIME - NTT)19,18,18
18 CALL PROUT(NUM,N,NTIME,M,MS,U,DELT,INDEX)
19 NTT = NTN + NTIME
19 IF(NTIME - NTOTL) 20,1,1
20 NTIME = NTIME + 1
GO TO 14

```

C FORMATS FOR INPUT AND OUTPUT STATEMENTS

```

100 FORMAT(2I3)
101 FORMAT(8F10.3)
102 FORMAT(13//,42X,'CLOTHING PARAMETERS',/,44X,'LAYER',2X,'MS',2X,'RESI
1STANCE',2X,'CAPACITANCE',/,56X,'(MIN/CM)',6X,'(CM)',/,)
201 FORMAT(46X,11,4X,12,3X,F6.3,6X,F8.2)
99 CALL EXIT
END

```

VARIABLE ALLOCATIONS

```

AIR )=0093-0000
VTIR )=0309-02FD
VAVEG(R )=038A
TNIR )=03CC
CS(R )=03DE
I(I )=03EF
MN(I )=03F5
KIN(I )=03FB
BIR )=0129-0096
MIR )=039F-030C
U(R )=03BD
TD(R )=03CF
Q(R )=03E1
NUM(I )=03F0
NK(I )=03F6
LIN(I )=03FC
CIR )=01BF-012C
MASS(R )=03AE-03A2
DECAY(R )=03C0
TRIR )=03D2
MS(I )=03E7-03E4
NTOTL(I )=03F1
NTT(I )=03F7
LTHLY(I )=03FD
R(R )=0255-01C2
RTHIN(R )=03B1
DELT(R )=03C3
RA1(R )=03D5
INDEX(I )=03EC-03E8
NTN(I )=03F2
NTIME(I )=03F8
NL(I )=03FE
VIR )=02EB-0258
VTHIN(R )=03B4
EFFIC(R )=03C6
RA2(R )=03D8
N(I )=03ED
NTD(I )=03F3
ITHLY(I )=03F9
LTHSL(I )=03FF
RT(R )=02FA-02EE
RAVEG(R )=03B7
TOTAL(R )=03C9
G(R )=03D8
NS(I )=03EE
NTR(I )=03F4
KTHSL(I )=03FA
NSURF(I )=0400

```

STATEMENT ALLOCATIONS

```

100 )=0409 101 )=040C 102 )=040F 200 )=0415 201 )=0448 1 )=046A 2 )=0475 3 )=04A6 14 )=0524 16 )=054A
17 )=0552 18 )=0558 19 )=0568 20 )=056E 99 )=0576

```

FEATURES SUPPORTED
ONE WORD INTEGERS
EXTENDED PRECISION
IOCS

CALLED SURPROGRAMS

```

AGENT INDX CONST CLOTH DECON PROUT ELD ESTO CARDZ PRNTZ SRED SWRT SCOMP SF10 SIOFX
SIOX SIOF SIOI SUBSC SDF10

```

INTFGR CONSTANTS

```

2=0404 1=0405 4=0406 0=0407 3=0408

```

CORE REQUIREMENTS FOR

```

COMMON 0 VARIABLES 1028 PROGRAM 372

```

END OF COMPILATION

// XEQ

A MATHEMATICAL MODEL FOR THE PENETRATION OF CLOTHING AND SKIN

TRANSFER OF VAPOUR THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING

SKIN TYPE - AVERAGE
RESISTANCE = 4.000 (MIN/CM)
CAPACITANCE = 375.0 (CM)

WINDSPEED = 6.87 (CM/SEC)
BOUNDARY LAYER RESISTANCE = 0.200 (MIN/CM)
DECOMPOSITION RATE = 0.003 (1/MIN)

CLOTHING PARAMETERS
LAYER MS RESISTANCE CAPACITANCE
(MIN/CM) (CM)

1	10	0.050	500.00
2	10	0.050	500.00

TIME CONSTANTS

TOTAL TIME = 30.00 (HOURS)
TIME OF DECONTAM = 0.00 (HOURS)
TIME INCREMENT = 1.00 (HOURS)
DELT = 0.100 (MINUTES)

SATURATED VAPOR CONCENTRATION
SVC = 0.1500E-03 (MG/CM**3)

INITIAL LIQUID LOADING

MASS IN LAYER 1	0.400	MG/CM**2
MASS IN LAYER 2	0.400	MG/CM**2
MASS ON SURFACE	0.400	MG/CM**2

MASS IN EACH LAYER IN MG/CM**2

TIME HOURS	U MG/CM**2	SYSTEMIC DOSE	MASS IN TRANSITIONAL LAYER	MASS IN HORNY LAYER	MASS IN FIRST CLOTH LAYER	MASS IN SECOND CLOTH LAYER
1.000	0.04495	0.000104	0.0105808	0.0550480	0.3051197	0.3865000
2.000	0.08991	0.0001746	0.0146571	0.0546033	0.2756698	0.3730001
3.000	0.13487	0.0006346	0.0168342	0.0546446	0.2468674	0.3595002
4.000	0.17983	0.0013504	0.0179844	0.0540895	0.2192642	0.3460002
5.000	0.22479	0.0022331	0.0185868	0.0535365	0.1919906	0.3325003
6.000	0.26975	0.0032130	0.0188659	0.0530523	0.1649487	0.3190004
7.000	0.31471	0.0042461	0.0189405	0.0525787	0.1381910	0.3055005
8.000	0.35967	0.0053056	0.0188870	0.0519900	0.1118331	0.2920005

LIQUID ALL GONE FROM SURFACE AT T= 8.89 (HOURS)

9.000	0.40463	0.0063757	0.0187499	0.0512754	0.0859523	0.2738547
-------	---------	-----------	-----------	-----------	-----------	-----------

LIQUID ALL GONE IN LAYER 1 AT T= 9.56 (HOURS)

10.000	0.44862	0.0074467	0.0185519	0.0504966	0.0707335	0.2062722
11.000	0.49015	0.0085124	0.0183080	0.0496954	0.0696731	0.1276530

LIQUID ALL GONE IN CLOTHING AT T= 11.75 (HOURS)

LAST SLICE TO CONTAIN LIQUID WAS 21

12.000	0.52858	0.0095687	0.0179982	0.0477028	0.0636273	0.0596048
13.000	0.55445	0.0106116	0.0140290	0.0343354	0.0442316	0.0387036
14.000	0.57191	0.0116201	0.0130115	0.0239987	0.0307725	0.0268091
15.000	0.58405	0.0125380	0.0101158	0.0167963	0.0215104	0.0187089
16.000	0.59253	0.0133176	0.0076603	0.0117903	0.0150864	0.0131069
17.000	0.59849	0.0139451	0.0056993	0.0082952	0.0106074	0.0092078
18.000	0.60267	0.0144320	0.0041882	0.0058466	0.0074726	0.0064824
19.000	0.60562	0.0148005	0.0030505	0.0041266	0.0052721	0.0045712
20.000	0.60770	0.0150745	0.0022074	0.0029157	0.0037239	0.0032276
21.000	0.60917	0.0152759	0.0015897	0.0020619	0.0026328	0.0022812
22.000	0.61221	0.0154225	0.0011406	0.0014590	0.0018627	0.0016135
23.000	0.61094	0.0155286	0.0008162	0.0010329	0.0013186	0.0011420
24.000	0.61146	0.0156051	0.0005828	0.0007316	0.0009338	0.0008086
25.000	0.61183	0.0156599	0.0004155	0.0005183	0.0006615	0.0005728
26.000	0.61209	0.0156991	0.0002959	0.0003673	0.0004687	0.0004058
27.000	0.61228	0.0157271	0.0002105	0.0002603	0.0003322	0.0002876
28.000	0.61241	0.0157571	0.0001496	0.0001845	0.0002355	0.0002038
29.000	0.61250	0.0157613	0.0001063	0.0001308	0.0001669	0.0001445

CLOTHING REPLACED AT T= 30.00 (HOURS)

30.000	0.61257	0.0157714	0.0000755	0.0000870	0.0000057	0.0000000
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// PAUS

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KEY WORDS

Systemic Dose
 Vapour Penetration
 Vapour Diffusion
 Protective Clothing
 Liquid Contamination

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